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SPATIAL AND MATERIAL STRESS TENSORS IN CONTINUUM
MECHANICS OF GROWING SOLID BODIES



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We presently derive generalized expressions of the stress tensor for continuum bodies with varying mass, considering both the Lagrangian and Eulerian viewpoints in continuum mechanics. We base our analysis and derivation of the expressions of both Cauchy and Eshelby stress tensors on an extension of the virial theorem for both discrete and continuous systems of material points with variable mass. The proposed framework is applicable to describe physical systems at very different scales, from the evolution of a population of biological cells accounting for growth to mass ejection phenomena occurring within a collection of gravitating objects at the very large astrophysical scales. As a starting basis, the field equations in continuum mechanics are written to account for a mass source and a mass flux, leading to a formulation of the virial theorem accounting for a varying mass within the considered system. The scalar and tensorial forms of the virial theorem are written successively in both Lagrangian and Eulerian formats, incorporating the mass flux. This delivers generalized formal expressions of Cauchy and Eshelby stress tensors versus the average tensor spatial and material virials respectively, incorporating the mass flux contribution.

1. Introduction

There are many problems in physics which involve masses changing with time, as exemplified by situation of growing bodies, solids and fluids exhibiting phase transitions [Ericksen 1984] related to solidification, evaporation, sedimentation. In particular, the mass balance (mass absorbency) influence phase transitions conditions, see for instance [dell'Isola and Iannece 1989; Eremeyev and Pietraszkiewicz 2009; 2011]. To mention but a few, two specific situations illustrate the very wide range of scales at which such phenomena may occur: growth or resorption in biological systems is a typical situation where the overall mass of a continuous body or a collection of particles varies, due to mass production within the system, or to a flux of mass through the system boundary. Growth at cellular level (individual

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cells can then be regarded as punctual masses) is typical of discrete growth, while the continuous aspect is of relevance for large collections of cells, organized within tissues for which the framework of continuous mechanics is adequate.

At a much larger scale, the dynamics of galaxies with mass loss due to either mass accretion or mass ablation has deserved a lot of attention in the literature for many years, usually relying on an extension of Newton's law of motion [Gommerstadt 2001], as originally stated by Sommerfeld in 1952.

In 1870, Rudolf Clausius [1870] stated that the mean *vis viva* of the system is equal to its *virial*, or that the average kinetic energy is equal to half the average potential energy. The virial theorem which was there born is a way to analyze the dynamics of a collection of interacting particles; it allows the average total kinetic energy to be calculated from the potential energy of a stable system. This holds even for very complicated systems that defy an exact solution, such as those considered in statistical mechanics or in astrophysics when considering large scales. Lord Rayleigh published a generalization of the virial theorem in 1903. Henri Poincaré applied a form of the virial theorem to the problem of determining the cosmological stability in 1911. A tensor form of the virial theorem was set up in [Chandrasekhar and Fermi 1953; Chandrasekhar and Lebovitz 1962; Parker 1954], both in the context of astrophysics.

The virial theorem has a rather broad physical significance; it has been extended to include electric and magnetic fields. The virial has both a discrete and a continuum facet, the first facet being well adapted to the physical situation of a finite collection of particles, while the continuum virial obtained by some kind of averaging process brings a simplification by introducing fields in place of discrete quantities. In the context of continuum mechanics, the virial theorem proves an alternative efficient manner to derive the pressure for particles without internal structure (fluids), avoiding thereby the — sometimes complex — derivation of a thermodynamic potential (the free energy).

The virial theorem has raised a renewed interest in the contemporary literature in relation to the construction of the Cauchy stress for structured media, derived from the tensorial virial theorem in [Jouanna and Brocas 2001; Jouanna and Pèdesseau 2004], borrowing arguments from statistical mechanics. The general idea at the root of the molecular definition of the average stress is the identification of molecules or atoms as interacting point masses. This reminds to the similar pioneering work of Irving and Kirkwood [1950], in which stress is defined as a pointwise statistical averaging performed in time instead of space, relying on the ergodicity hypothesis. This viewpoint applies for a number of molecules which is large enough for averaging operations to make sense — instead of using quantum mechanics — so that a classical description can be adopted. Works in the literature since this pioneering contribution witness a diversity of definitions and derivations

of the stress tensor using a molecular viewpoint, see the recent critical overview [Murdoch 2007] and references therein. Especially, when micro-macro identification processes are considered, higher gradient theories naturally arise in which to Cauchy stress tensor one needs to add a family of hyper stresses, as already remarked by Gabrio Piola in his pioneering works [dell'Isola and Iannece 1989; dell'Isola et al. 2012; 2014].

As a main outcome and novelty of the present contribution, one shall derive expressions of the material Eshelby stress and spatial Cauchy stress tensors for continuum bodies witnessing a local change of their mass. We base our analysis and derivation of the expressions of both Cauchy and Eshelby stress tensors on an extension of the virial theorem for both discrete and continuous systems of material points with variable mass, thereby generalizing developments exposed in [Ganghoffer 2010b]. Eshelby stress appears as a driving force for the growth of continuum solid bodies, possibly incorporating multiphysical phenomena, see [Ganghoffer 2010a; 2012].

The present contribution is organized as follows. In order to set the stage, the virial theorem is first recalled in both scalar and tensorial formats (Section 2). We next extend in Section 3 the virial theorem for systems with variable mass, a situation which occurs for growing biological systems and for a set of gravitational masses with mass loss at the other extreme of the length spectrum. The virial theorem for systems with variable mass is derived in sections 2 and 3 in Eulerian format, and the material counterpart is written in sections 4 and 5, highlighting the variation of the average virial in relation to the divergence of Eshelby stress. A summary of the main developments is given in Section 6.

A few words regarding notation are in order. Vectors and higher-order tensors are denoted with boldface symbols. Likewise, tensorial quantities built from their scalar counterparts are denoted as boldface characters with a superposed hat; e.g., $\hat{\mathbf{E}}_k$ denotes the tensorial kinetic energy, such that its trace is the scalar kinetic energy: $\text{Tr}(\hat{\mathbf{E}}_k) = E_k$. The summation convention on repeated indices is in force, unless otherwise explicitly stated.

The bracket $\langle \cdot \rangle$ denotes the ensemble average of any quantity. The partial derivative of a scalar function $f(x)$ is denoted $\partial_x f = \partial f / \partial x$; the time derivative of a function $\mathbf{a}(t)$ is represented by a superposed dot: $\dot{\mathbf{a}}(t) = d\mathbf{a}(t)/dt$. The material and spatial gradients are denoted $\text{Grad} \equiv \nabla_R$ and $\text{grad} \equiv \nabla$ respectively; similarly, the material and spatial divergence are denoted $\text{Div}(\cdot) \equiv \nabla_R(\cdot)$ and $\text{div}(\cdot) = \nabla \cdot (\cdot)$ respectively. The transpose of the linear mapping A is the linear mapping denoted A^T . The notation $\text{sym}(\cdot)$ stands for the symmetrized part of a dyadic product. The second-order identity tensor is denoted \mathbf{I} .

Nomenclature of the principal symbols

\mathbf{R}, \mathbf{R}_i (\mathbf{r}, \mathbf{r}_i)	material (resp. spatial) position vectors
\mathbf{J}	inertia tensor
$\mathbf{p}_i := m_i \dot{\mathbf{r}}_i$	momentum of a single particle
\hat{V}, \hat{V}	scalar and tensorial virials ; $\hat{V}_{\text{int}}, \hat{V}_{\text{ext}}$ internal and external scalar virials
$\langle \cdot \rangle$	ensemble averaging (equivalent to time averaging according to ergodicity)
$\langle \hat{V}_0 \rangle$ (resp. $\langle \hat{V}_0 \rangle$)	average scalar (resp. tensorial) material virial
$\langle \hat{V} \rangle$ (resp. $\langle \hat{V} \rangle$)	average scalar (resp. tensorial) spatial virial
E_k, E_p	kinetic and potential energy respectively
\hat{E}_k, \hat{E}_p	tensorial kinetic and potential energy respectively
$\mathbf{F} := \text{Grad } \mathbf{r}$	first-order transformation gradient
$\mathbf{J} := \det(\mathbf{F})$	
ψ	kinematically admissible position field
f_0, \mathbf{f}	referential and spatial body forces
${}^3\mathbf{G} := \nabla_X \mathbf{F}$	second-order transformation gradient
$W_0(\mathbf{F})$	strain energy density
$\mathbf{T} := \partial W_0(\mathbf{F}) / \partial \mathbf{F}$	first Piola–Kirchhoff stress
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\Sigma} := W_0 \mathbf{I} - \mathbf{F}^t \cdot \mathbf{T}$	second-order Eshelby stress
$\tilde{\boldsymbol{\Sigma}} := W_0 \mathbf{I}^4 - \mathbf{F}^t \otimes \mathbf{T}$	fourth-order Eshelby stress

2. Scalar and tensorial virial theorems for systems with constant mass

In order to set the stage, a reminder of the statement of the virial theorems in both scalar and tensorial format for systems of particles with constant mass are conveniently recalled.

The Lagrangian of a set of N point particles with mass m_i and position vector \mathbf{r}_i , moving in a potential $E_p(\{\mathbf{r}_i\})$, is the difference between the kinetic energy

$$E_k(\{\dot{\mathbf{r}}_i\}) := \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_i}, \quad (2-1)$$

where $\mathbf{p}_i := m_i \dot{\mathbf{r}}_i$ is the momentum of the i -th particle, and the potential energy:

$$L(\{\mathbf{r}_i, \dot{\mathbf{r}}_i\}) := E_k(\{\dot{\mathbf{r}}_i\}) - E_p(\{\mathbf{r}_i\}). \quad (2-2)$$

In the hamiltonian formulation, the independent variables are the spatial positions and the momenta, namely the set of variables $\{\mathbf{r}_i, \mathbf{p}_i\}$. The Lagrangian is related

to the Hamiltonian

$$H(\{\mathbf{r}_i, \mathbf{p}_i\}) := E_k + E_p, \quad (2-3)$$

defined as the sum of the kinetic and potential energies of the individual particles, by the equation

$$L(\mathbf{r}, \dot{\mathbf{r}}; t) = \mathbf{p} \cdot \frac{d\mathbf{r}}{dt} - H(\mathbf{r}, \mathbf{p}; t). \quad (2-4)$$

Each material point is submitted to a force given by the gradient of the potential energy vs. the corresponding spatial position, hence

$$\mathbf{f}_i = -\partial_{\mathbf{r}_i} E_p. \quad (2-5)$$

The scalar virial theorem states that the virial, viz the scalar valued quantity

$$\hat{V} := \sum_{i=1}^N \mathbf{r}_i \cdot \mathbf{f}_i \quad (2-6)$$

is related to the kinetic energy of the set of particles by (the arguments of the functionals are omitted for the sake of simplicity)

$$\frac{d}{dt} \left(\sum_{i=1}^N \mathbf{p}_i \cdot \mathbf{r}_i \right) = 2E_k + \hat{V}. \quad (2-7)$$

In the asymptotic limit of infinite times, the time average — indicated by the bracket operator — of the left side of the previous identity vanishes, hence the ensemble average of the right side vanishes:

$$2\langle E_k \rangle + \langle \hat{V} \rangle = 0. \quad (2-8)$$

This identity constitutes the scalar version of the virial theorem. The assumption of ergodicity at the macroscopic equilibrium implies that time averages at fixed coordinate (following a single particle) are interchangeable with ensemble averages (averages over a sufficiently large set of particles) at fixed time.

The virial can be decomposed into the sum of the internal virial \hat{V}_{int} and the external virial \hat{V}_{ext} , as

$$\hat{V} = (\mathbf{f}_{ij} \cdot \mathbf{r}_{ij})_{j \neq i} + \mathbf{f}_{i,\text{ext}} \cdot \mathbf{r}_i \equiv \hat{V}_{\text{int}} + \hat{V}_{\text{ext}} \quad (2-9)$$

highlighting the contribution of internal forces \mathbf{f}_{ij} (first term on the right due to interparticle interactions) and external forces (body forces due to gravity and contact), denoted $\mathbf{f}_{i,\text{ext}}$, adopting the notation $\mathbf{r}_{ij} := \mathbf{r}_i - \mathbf{r}_j$ for the relative position of particles i and j .

The generalized virial theorem established in [Jouanna and Brocas 2001], viz the tensorial generalization of the identities (2-6), (2-7), (2-8), can be obtained as

follows: let differentiate twice the (symmetrical) inertia tensor (the summation of repeated indices in the dyadic products is done over the set of N particles)

$$\mathbf{I} := m_i \mathbf{r}_i \otimes \mathbf{r}_i \quad (2-10)$$

hence giving

$$\frac{d\mathbf{I}}{dt} := m_i (\dot{\mathbf{r}}_i \otimes \mathbf{r}_i + \mathbf{r}_i \otimes \dot{\mathbf{r}}_i)$$

and so

$$\frac{d^2\mathbf{I}}{dt^2} = 2m_i \dot{\mathbf{r}}_i \otimes \dot{\mathbf{r}}_i + m_i (\ddot{\mathbf{r}}_i \otimes \mathbf{r}_i + \mathbf{r}_i \otimes \ddot{\mathbf{r}}_i) = 2\hat{\mathbf{E}}_k + \hat{\mathbf{V}}, \quad (2-11)$$

with

$$\hat{\mathbf{V}} := 2 \text{sym}(\mathbf{r}_i \otimes \mathbf{f}_i) = -2 \text{sym}(\mathbf{r}_i \otimes \partial_{\mathbf{r}_i} E_p) \quad (2-12)$$

defined as the tensorial virial, and the tensorial kinetic energy elaborated as

$$\hat{\mathbf{E}}_k := 2m_i \dot{\mathbf{r}}_i \otimes \dot{\mathbf{r}}_i \equiv \frac{\mathbf{p}_i \otimes \mathbf{p}_i}{2m_i}. \quad (2-13)$$

Remark. The trace of $\hat{\mathbf{V}}$ gives the scalar virial, $\text{Tr}(\hat{\mathbf{V}}) = \hat{\mathbf{V}}$; similarly, the scalar kinetic energy is recovered as the trace of its tensorial generalization.

Considering the asymptotic limit of infinite times, the identity (2-11) further gives the generalized (tensorial) virial theorem, as the tensorial extension of the scalar virial theorem

$$2\langle \hat{\mathbf{E}}_k \rangle + \langle \hat{\mathbf{V}} \rangle = \mathbf{0}. \quad (2-14)$$

The virial can be decomposed into the sum of the internal virial $\hat{\mathbf{V}}_{\text{int}}$ and the external virial $\hat{\mathbf{V}}_{\text{ext}}$, as

$$\hat{\mathbf{V}} = (\mathbf{f}_{ij} \cdot \mathbf{r}_{ij})_{j \neq i} + \mathbf{f}_{i,\text{ext}} \cdot \mathbf{r}_i \equiv \hat{\mathbf{V}}_{\text{int}} + \hat{\mathbf{V}}_{\text{ext}} \quad (2-15)$$

highlighting the contribution of internal forces \mathbf{f}_{ij} (first term on the right due to interparticle interactions) and external forces (body forces due to gravity and contact), denoted $\mathbf{f}_{i,\text{ext}}$, adopting the notation $\mathbf{r}_{ij} := \mathbf{r}_i - \mathbf{r}_j$ for the relative position of particles i and j .

3. Scalar and tensorial virial theorems for systems with varying mass

Variable mass problems have been treated in the literature in the context of the virial theorem [Gommerstadt 2001], especially considering applications in astronomy. The authors especially mention that when a body is losing mass isotropically, no additional force should appear, thus the motion of the body will overall not be altered by mass losses.

The mass balance writes in integral form as

$$\frac{D}{Dt} \int_{\Omega} \rho \, dx = \int_{\Omega} \rho (\pi - \operatorname{div} \mathbf{J}) \, dx \quad (3-1)$$

in presence of a source term π and a mass flux vector \mathbf{J} , which can be identified for an open system including different chemical species as

$$\pi = \sum_k \rho_k \dot{n}_k, \quad \mathbf{J} = \sum_k \mathbf{J}_k. \quad (3-2)$$

In continuum mechanics, the balance of linear momentum is written in integral form as

$$\begin{aligned} \frac{D}{Dt} \int_{\Omega} \rho \mathbf{v} \, dx &= \int_{\Omega} \mathbf{f} \, dx + \int_{\partial\Omega} \mathbf{n} \cdot \boldsymbol{\sigma} \, ds + \int_{\Omega} \pi \mathbf{v} \, dx - \int_{\partial\Omega} \mathbf{n} \cdot (\mathbf{J} \otimes \mathbf{v}) \, ds \\ &= \int_{\Omega} \mathbf{f} \, dx + \int_{\partial\Omega} \mathbf{n} \cdot \boldsymbol{\sigma} \, ds + \int_{\Omega} \pi \mathbf{v} \, dx - \int_{\Omega} \operatorname{div}(\mathbf{v} \otimes \mathbf{J}) \, dx \\ &\equiv \int_{\Omega} \mathbf{f} \, dx + \int_{\Omega} \pi \mathbf{v} \, dx + \int_{\Omega} \operatorname{div}(\boldsymbol{\sigma} - \mathbf{v} \otimes \mathbf{J}) \, dx. \end{aligned} \quad (3-3)$$

The last equality highlights that the effective stress is in fact the second order tensor

$$\tilde{\boldsymbol{\sigma}} := \boldsymbol{\sigma} - \mathbf{v} \otimes \mathbf{J}.$$

Note that we have used the fact the divergence is presently elaborated as the right divergence operator. For a continuum body, the strong form of the mass and momentum balance laws in presence of mass changes are successively obtained as

$$\frac{d\rho}{dt} \equiv \dot{\rho} = \pi - \nabla \cdot \mathbf{J} - \rho \nabla \mathbf{v} \quad (3-4)$$

and

$$\rho \frac{d\mathbf{v}}{dt} = \mathbf{f} + \nabla \cdot \boldsymbol{\sigma} - (\mathbf{J} \cdot \nabla) \mathbf{v} \equiv \mathbf{f} + \nabla \cdot \boldsymbol{\sigma} - \nabla \mathbf{v} \cdot \mathbf{J},$$

that is to say

$$\begin{aligned} \rho \frac{dv_i}{dt} &= f_i + \sigma_{ip,p} - \frac{\partial v_i}{\partial x_p} J_p \\ &= f_i + \sigma_{ip,p} - J_p v_{i,p} = f_i + (\sigma_{ip} - v_i J_p)_{,p} + v_i \operatorname{div} \mathbf{J}. \end{aligned}$$

This entails the balance of linear momentum equality

$$\rho \frac{d\mathbf{v}}{dt} = (\mathbf{f} + \mathbf{v} \operatorname{div} \mathbf{J}) + \nabla \cdot \tilde{\boldsymbol{\sigma}}. \quad (3-5)$$

We can see that the additional contribution $\mathbf{v} \operatorname{div} \mathbf{J}$ acts in fact as a source term in the balance of linear momentum (3-5), and can be incorporated into the overall effective body force, quantity $(\mathbf{f} + \mathbf{v} \operatorname{div} \mathbf{J})$.

3.1. Cauchy stress from the discrete form of the virial theorem. The discrete scalar virial in eulerian form is built as the dyadic product of the spatial positions of the material points with the forces acting on them [Jouanna and Brocas 2001]:

$$\hat{V} = \sum_{i=1}^N \mathbf{r}_i \cdot \mathbf{f}_i = \sum_{i,j=1}^N (\mathbf{f}_{ij} \cdot \mathbf{r}_{ij})_{j \neq i} + \sum_{i=1}^{N_{\text{ext}}} \mathbf{f}_{i,\text{ext}} \cdot \mathbf{r}_i \equiv \hat{V}_{\text{int}} + \hat{V}_{\text{ext}},$$

yielding

$$\begin{aligned} \langle \hat{V} \rangle &= \langle \hat{V}_{\text{int}} \rangle + \langle \hat{V}_{\text{ext}} \rangle \cong \left\langle \sum_{i=1}^{N_{\text{con}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{con}} \right\rangle + \left\langle \sum_{i=1}^{N_{\text{ext}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{vol}} \right\rangle \\ &= \int_{\partial\Omega} \mathbf{r} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} \, d\sigma_t + \int_{\Omega} \mathbf{r} \cdot \mathbf{f} \, dx \\ &= \int_{\Omega} (\mathbf{r} \cdot \text{div } \boldsymbol{\sigma} + \boldsymbol{\sigma}^t : \text{grad } \mathbf{r}) \, dx + \int_{\Omega} \mathbf{r} \cdot \mathbf{f} \, d\sigma_t \\ &= \int_{\Omega} (\mathbf{r} \cdot \text{div } \boldsymbol{\sigma} + \boldsymbol{\sigma}^t : \mathbf{I}) \, dx + \int_{\Omega} \mathbf{r} \cdot \mathbf{f} \, dx \end{aligned} \quad (3-6)$$

which we view as the ensemble average of the discrete (scalar) eulerian virial, denoted by $\langle V \rangle$. Since contact and external (body) forces do not act on the same material points, we have indicated in (3-6) the range of these respective material points by N_{cont} and N_{ext} , respectively; this notation will be retained throughout.

The contribution $\int_{\partial\Omega} \mathbf{r} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} \, d\sigma_t$ in previous equality represents the exterior virial due to contact forces, considering that interactions between particles have a very short range, hence the particles contributing to the external virial are those located near the boundaries of the considered volume element. These forces are in fact contact forces (reflected in the existence of Cauchy stress at the continuum level), and thus are considered as internal forces corresponding to the internal virial \hat{V}_{int} . The contribution $\int_{\Omega} \mathbf{r} \cdot \mathbf{f} \, d\sigma_t$ represents the contribution to the scalar virial due to external forces, and is accordingly coined the *external virial*, denoted \hat{V}_{ext} in (3-6).

In the sequence of equalities in (3-6), we have used the analogy between the discrete and continuous counterpart of the scalar virial of external and contact (internal) forces. The second row of equalities in (3-6) is the continuous counterpart of the discrete elaboration of the scalar virial in (2-6), as previously explained: internal forces in a continuum mechanical description are identified to contact forces, while external forces are typically body forces or any force at distance.

Introducing therein the previous balance of momentum, rewritten here for the sake of clarity as

$$\rho \frac{d\mathbf{v}}{dt} = \mathbf{f} + \nabla \cdot \boldsymbol{\sigma} - (\mathbf{J} \cdot \nabla) \mathbf{v}$$

leads further to

$$\left\langle \sum_{i=1}^{N_{\text{cont}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{con}} \right\rangle + \left\langle \sum_{i=1}^{N_{\text{ext}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{vol}} \right\rangle = \int_V \mathbf{r} \cdot (\rho \boldsymbol{\gamma} + (\mathbf{J} \cdot \nabla) \mathbf{v}) dV + \int_V \boldsymbol{\sigma}^T : \mathbf{I} dV. \quad (3-7)$$

Introducing the acceleration $\boldsymbol{\gamma} := d\mathbf{v}/dt$ therein. One can thus express the trace of Cauchy stress as

$$\begin{aligned} |V|I_1(\boldsymbol{\sigma}) &:= |V| \text{Tr}(\boldsymbol{\sigma}) \\ &= \left\langle \sum_{i=1}^{N_{\text{cont}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{con}} \right\rangle + \left\langle \sum_{i=1}^{N_{\text{ext}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{vol}} \right\rangle - \int_V \mathbf{r} \cdot (\rho \boldsymbol{\gamma} + (\mathbf{J} \cdot \nabla) \mathbf{v}) dV \\ &\cong \left\langle \sum_{i=1}^{N_{\text{cont}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{con}} \right\rangle + \left\langle \sum_{i=1}^{N_{\text{ext}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{vol}} \right\rangle - \int_V \mathbf{r} \cdot (\mathbf{J} \cdot \nabla) \mathbf{v} dV. \end{aligned} \quad (3-8)$$

It is customary to neglect the inertia forces, so that the pressure now involves an additional contribution given by the last integral in previous equality, involving the mass flux. The last equality is the extended scalar virial theorem in Eulerian format accounting for mass changes within a body of a set of particles.

The tensor form of the virial theorem is obtained as follows:

$$\begin{aligned} \mathbf{V}_{\text{ext,tot}} &= \mathbf{V}_{\text{ext,con}} + \mathbf{V}_{\text{ext,vol}} \cong \left\langle \sum_{i=1}^{N_{\text{cont}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{con}} \right\rangle + \left\langle \sum_{i=1}^{N_{\text{ext}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{vol}} \right\rangle \\ &= \int_{\partial V} \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} ds + \int_V \mathbf{r} \otimes \mathbf{f}_{\text{vol}} dx \\ &= \int_V (\mathbf{r} \otimes \text{div} \boldsymbol{\sigma} + \mathbf{I} \cdot \boldsymbol{\sigma}^T) dx + \int_V \mathbf{r} \otimes \mathbf{f}_{\text{vol}} dx. \end{aligned} \quad (3-9)$$

Inserting the previous balance of linear momentum delivers the equality

$$\begin{aligned} &\left\langle \sum_{i=1}^{N_{\text{cont}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{con}} \right\rangle + \left\langle \sum_{i=1}^{N_{\text{ext}}} \mathbf{r}_i \cdot \mathbf{f}_{i,\text{vol}} \right\rangle \\ &= \int_V (\mathbf{r} \otimes (\rho \boldsymbol{\gamma} - \mathbf{f} + (\mathbf{J} \cdot \nabla) \mathbf{v}) + \boldsymbol{\sigma}^T) dx + \int_V \mathbf{r} \otimes \mathbf{f}_{\text{vol}} dx. \end{aligned} \quad (3-10)$$

Neglecting body forces on both sides and inertia forces we can then obtain the average of the Cauchy stress tensor:

$$\int_V \boldsymbol{\sigma}^T dx \approx |V| \bar{\boldsymbol{\sigma}}^T = \left\langle \sum_{i=1}^N \mathbf{r}_i \otimes \mathbf{f}_{i,\text{con}} \right\rangle - \int_V (\mathbf{r} \otimes (\rho \boldsymbol{\gamma} - \mathbf{f} + (\mathbf{J} \cdot \nabla) \mathbf{v})) dx,$$

leading to

$$\boldsymbol{\sigma}^T = \frac{1}{|V|} \left\langle \sum_{i=1}^{N_{\text{cont}}} \mathbf{r}_i \otimes \mathbf{f}_{i,\text{con}} \right\rangle - \frac{1}{|V|} \int_V \mathbf{r} \otimes (\mathbf{J} \cdot \nabla) \mathbf{v} \, dx. \quad (3-11)$$

We have considered a small enough volume so that the stress tensor can be considered as homogeneous inside. Thereby, Cauchy stress tensor is expressed versus the average virial of contact forces and the additional contribution of mass flux, in identified as the last integral in previous equality.

The average Cauchy stress can alternatively be derived from the continuum version of the virial theorem, as exposed in the next subsection. We shall in addition and as a matter of completeness incorporate the inertia forces, which have been neglected in previous derivations.

3.2. Continuum form of the virial theorem and average Cauchy stress. The full derivation of the virial theorem in scalar format and from a purely continuum viewpoint (that is without resorting to the discrete mechanics of a set of interacting particles) delivers the average of Cauchy stress as an extension of the virial theorem with constant mass (see for example identity (3) in [Gommerstadt 2001]) as

$$\frac{1}{|V|} \int_V \boldsymbol{\sigma} \, dx = \frac{1}{|V|} \mathbf{E}_c - \frac{1}{2|V|} \frac{d^2 \mathbf{I}}{dt^2} + \frac{1}{2|V|} \int_{\partial V} \mathbf{x} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} \, ds. \quad (3-12)$$

The tensor of kinetic energy therein is defined as

$$\mathbf{E}_c := \frac{1}{2} \int_V \rho \mathbf{v} \otimes \mathbf{v} \, dx. \quad (3-13)$$

The inertia tensor and its second material derivative are computed successively as follows:

$$\begin{aligned} \mathbf{I} &= \int_V \rho \mathbf{x} \otimes \mathbf{x} \, dx \\ \frac{d\mathbf{I}}{dt} &= \int_V \rho (\mathbf{x} \otimes \mathbf{v} + \mathbf{v} \otimes \mathbf{x}) \, dx + \int_V \frac{d\rho}{dt} \mathbf{x} \otimes \mathbf{x} \, dx + \int_V \rho (\mathbf{x} \otimes \mathbf{x}) \nabla \cdot \mathbf{v} \, dx \\ \frac{d^2 \mathbf{I}}{dt^2} &= \int_V \rho (\boldsymbol{\gamma} \otimes \mathbf{x} + \mathbf{x} \otimes \boldsymbol{\gamma} + 2\mathbf{v} \otimes \mathbf{v}) \, dx + 2 \int_V (\dot{\rho} + \rho \nabla \cdot \mathbf{v}) \frac{D}{Dt} (\mathbf{x} \otimes \mathbf{x}) \, dx \\ &\quad + \int_V \left(\ddot{\rho} + 2\dot{\rho} \nabla \cdot \mathbf{v} + \rho \frac{D}{Dt} (\nabla \cdot \mathbf{v}) + \rho (\nabla \cdot \mathbf{v})^2 \right) (\mathbf{x} \otimes \mathbf{x}) \, dx. \end{aligned} \quad (3-14)$$

In the particular case of incompressible media, the condition $\nabla \cdot \mathbf{v} = 0$ entails the simplified expression of the second-order material derivative of the inertia tensor

$$\frac{d^2 \mathbf{I}}{dt^2} = \int_V \rho (\boldsymbol{\gamma} \otimes \mathbf{x} + \mathbf{x} \otimes \boldsymbol{\gamma} + 2\mathbf{v} \otimes \mathbf{v}) \, dx + 2 \int_V \dot{\rho} \frac{D}{Dt} (\mathbf{x} \otimes \mathbf{x}) \, dx + \int_V \ddot{\rho} (\mathbf{x} \otimes \mathbf{x}) \, dx \quad (3-15)$$

in which the second-order time derivative of the mass density results from balance law (3-4) incorporating mass source and mass flux contributions.

Inserting expression (3-14) into (3-12) then delivers the following expression for the average Cauchy stress tensor:

$$\begin{aligned}
 \bar{\boldsymbol{\sigma}} &:= \frac{1}{|V|} \int_V \boldsymbol{\sigma} \, dx \\
 &= \frac{1}{|V|} \mathbf{E}_c + \frac{1}{2|V|} \int_{\partial V} \mathbf{x} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} \, ds \\
 &\quad - \frac{1}{2|V|} \left\{ \int_V \rho (\boldsymbol{\gamma} \otimes \mathbf{x} + \mathbf{x} \otimes \boldsymbol{\gamma} + 2\mathbf{v} \otimes \mathbf{v}) \, dx + 2 \int_V (\dot{\rho} + \rho \nabla \cdot \mathbf{v}) \frac{D}{Dt} (\mathbf{x} \otimes \mathbf{x}) \, dx \right. \\
 &\quad \left. + \int_V \left(\ddot{\rho} + 2\dot{\rho} \nabla \cdot \mathbf{v} + \rho \frac{D}{Dt} (\nabla \cdot \mathbf{v}) + \rho (\nabla \cdot \mathbf{v})^2 \right) (\mathbf{x} \otimes \mathbf{x}) \, dx \right\}. \quad (3-16)
 \end{aligned}$$

Based on (3-15), this expression simplifies for incompressible media to deliver the full Cauchy stress tensor in averaged form:

$$\begin{aligned}
 \bar{\boldsymbol{\sigma}} &:= \frac{1}{|V|} \int_V \boldsymbol{\sigma} \, dx \\
 &= \frac{1}{|V|} \mathbf{E}_c + \frac{1}{2|V|} \int_{\partial V} \mathbf{x} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} \, ds \\
 &\quad - \frac{1}{2|V|} \left\{ \int_V \rho (\boldsymbol{\gamma} \otimes \mathbf{x} + \mathbf{x} \otimes \boldsymbol{\gamma} + 2\mathbf{v} \otimes \mathbf{v}) \, dx \right. \\
 &\quad \left. + 2 \int_V \dot{\rho} \frac{D}{Dt} (\mathbf{x} \otimes \mathbf{x}) \, dx + \int_V \ddot{\rho} (\mathbf{x} \otimes \mathbf{x}) \, dx \right\}. \quad (3-17)
 \end{aligned}$$

4. Material version of the scalar virial theorem for systems with varying mass

Since Cauchy stress represents a *spatial measure* of the contact forces in condensed matter, one expects a similar interpretation of the Eshelby stress, from the tensorial virial and extensions thereof, viewed as the *material counterpart* of Cauchy stress. Microscopic interpretations of the notion of Eshelby stress are of high interest, since this tensor leads to the so called material forces accounting for the presence of defects (inhomogeneities, such as inclusions or cracks) in material space [Maugin 1993]. Hence, discrete simulations in the configuration of the defects based on the virial can be conceived as a mean to evaluate those material forces at the very scale of the defect themselves.

Pursuing further along this line of thoughts, the construction of Eshelby stress from considerations tied to a system of discrete interacting punctual masses proves

also relevant in the context of the so-called continuum-atomistic modeling strategies in multiscale simulation methods, see [Alibert et al. 2003; Sunyk and Steinmann 2003; Tadmor et al. 1996] and references therein. Such an interpretation of the stress tensor has been done in the continuum modeling of granular materials such as sands, cements, clays, concrete, rocks and certain polymers [Misra and Singh 2015; Misra and Poorsolhjoui 2015b; 2015a].

We establish the material version of the scalar virial theorem; we adopt as for the eulerian situation a quasi-static framework, and define the scalar material virial \hat{V}_0 with ensemble average $\langle \hat{V}_0 \rangle$ as [Ganghoffer 2010b]

$$\begin{aligned} \langle \hat{V}_0 \rangle &:= - \int_{\partial \Omega_0} \mathbf{R} \cdot \boldsymbol{\Sigma} \cdot \mathbf{N} \, d\sigma_0 + \int_{\Omega_0} \mathbf{R} \cdot \mathbf{f}_R \, dX \\ &\equiv - \int_{\Omega_0} \mathbf{I} : \boldsymbol{\Sigma}^t \, dX \cong - \text{Tr}(\boldsymbol{\Sigma})|_{\Omega_0} \end{aligned} \quad (4-1)$$

considering a small enough volume element Ω_0 , so that the fields can be considered as nearly homogeneous (equilibrium in terms of Eshelby stress has been used); vector \mathbf{R} is the material position. Previous identity has been obtained by a pull-back of the eulerian form of the balance of linear momentum on the material manifold.

An elaboration of the scalar material virial can be done alternatively starting from a construction similar to that of the eulerian scalar virial in (2-6) for its discrete version or in (3-6) for the continuum counterpart: we define the scalar material virial as the dot product of the spatial positions of material points with the forces acting on them (with a change of sign for the internal virial of contact forces); developments presented in [Ganghoffer 2010b] lead to

$$\hat{V}_R = \sum_{i=1}^N \mathbf{R}_i \cdot \mathbf{f}_{Ri},$$

which is equivalent to

$$\begin{aligned} \langle \hat{V}_R \rangle &:= - \int_{\partial \Omega_R} \mathbf{R} \cdot \boldsymbol{\Sigma} \cdot \mathbf{N} \, d\sigma_R + \int_{\Omega} \mathbf{R} \cdot \mathbf{f}_R \, dX \\ &= - \int_{\Omega} (\mathbf{R} \cdot \nabla_R \cdot \boldsymbol{\Sigma} + \boldsymbol{\Sigma}^t : \nabla_R \mathbf{R}) \, dx + \int_{\Omega} \mathbf{R} \cdot \mathbf{f}_R \, d\sigma_t \\ &= - \int_{\Omega} (\mathbf{R} \cdot \nabla_R \cdot \boldsymbol{\Sigma} + \boldsymbol{\Sigma}^t : \mathbf{I}) \, dx + \int_{\Omega} \mathbf{R} \cdot \mathbf{f}_R \, dx. \end{aligned} \quad (4-2)$$

In previous set of equalities, the index R refers to the referential configuration; thus one has the identity $\hat{V}_R = \hat{V}_0$.

Inserting the material divergence of the Eshelby tensor $\boldsymbol{\Sigma}$, previously obtained as

$$\nabla_R \cdot \boldsymbol{\Sigma} = \nabla_R \cdot \tilde{\boldsymbol{\Sigma}} + \mathbf{J}_R \cdot \nabla_R \mathbf{F} \cdot \mathbf{v} + \nabla_R \cdot (\mathbf{F}^T \cdot (\mathbf{J}_R \otimes \mathbf{v})), \quad (4-3)$$

delivers the trace of Eshelby stress as

$$\begin{aligned} -|\Omega| \text{Tr}(\Sigma^T) &= \int_{\Omega} (\mathbf{R} \cdot \nabla_R \cdot \Sigma) dx + \int_{\Omega} \mathbf{R} \cdot \mathbf{f}_R dx - \langle \hat{V}_R \rangle \\ &= \int_{\Omega} (\mathbf{R} \cdot \nabla_R \cdot \tilde{\Sigma}) dx + \int_{\Omega} \mathbf{R} \cdot \{ \mathbf{J}_R \cdot \nabla_R \mathbf{F} \cdot \mathbf{v} + \nabla_R \cdot (\mathbf{F}^T \cdot (\mathbf{J}_R \otimes \mathbf{v})) \} dx \\ &\quad + \int_{\Omega} \mathbf{R} \cdot \mathbf{f}_R dx - \langle \hat{V}_R \rangle. \end{aligned}$$

Inserting therein the balance of momentum with the effective Eshelby stress finally delivers the trace of Eshelby stress versus the source of mass terms, the referential scalar virial, and the heat and chemical contributions:

$$\begin{aligned} -|\Omega| \text{Tr}(\Sigma^t) &= - \int_{\Omega} (\mathbf{R} \cdot \{ \Pi \mathbf{F}^T \cdot \mathbf{v} + \nabla_R \cdot [\mathbf{F}^T \cdot \tilde{\mathbf{T}}] + s \nabla_R \theta + \mu_k \nabla_R n_k \}) dx \\ &\quad + \int_{\Omega} \mathbf{R} \cdot \{ \nabla_R \cdot (\mathbf{F}^T \cdot (\mathbf{J}_R \otimes \mathbf{v})) \} dx - \langle \hat{V}_R \rangle. \quad (4-4) \end{aligned}$$

Microscopic interpretations of the notion of Eshelby stress are of high interest, since this tensor leads to the so-called material forces accounting for the presence of defects (inhomogeneities, such as inclusions or cracks) in material space [Maugin 1993]. Hence, discrete simulations in the configuration of the defects based on the virial can be conceived as a mean to evaluate those material forces at the very scale of the defect themselves. Since the virial relies on the consideration of a discrete set of interacting particles, one may further evoke the mixed continuum-atomistic approaches that prove adequate in nanomechanics, which combine the usual framework of continuum mechanics with a full atomic scale description based on interatomic potentials. The full Eshelby stress shall be derived in the next section from the virial theorem.

5. Eshelby stress for continua with variable mass

Recall that the tensorial virial states [Jouanna and Brocas 2001] that the transpose of the Cauchy stress may be expressed as the average external virial tensor divided by the volume occupied by the set of considered particles. The external tensorial virial is defined as the contribution of the tensorial virial due exclusively to the external forces $\mathbf{f}_{i,\text{ext}}$:

$$\hat{V}_{\text{ext}} := \mathbf{r}_i \otimes \mathbf{f}_{i,\text{ext}}. \quad (5-1)$$

It is the principal aim of this section to give a similar microscopic interpretation of the purely material Eshelby stress in terms of the material counterpart of the tensorial virial, to be elaborated in the sequel.

Starting from the tensorial eulerian virial as the following integral [Jouanna and Brocas 2001], adopting the continuum limit, viz

$$\langle \hat{V} \rangle \equiv \int_{\partial \Omega} \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} d\sigma_t + \int_{\Omega} \mathbf{r} \otimes \mathbf{f} dx. \quad (5-2)$$

And accounting for the relation between the spatial and material tensorial virials

$$\langle \hat{V} \rangle = \langle \hat{V}_0 \rangle + \int_{\Omega_0} W_0 \mathbf{I} dX \quad (5-3)$$

one obtains after length developments presented in the Appendix B the average of the Eshelby stress versus the eulerian tensorial virial:

$$\langle \hat{V} \rangle = \int_{\Omega_0} (-\text{tr}(\tilde{\boldsymbol{\Sigma}}^t) + W_0 \mathbf{I}) dX + \int_{\Omega_0} \mathbf{R} \cdot \left\{ \mathbf{F}^T \otimes \rho J \frac{d\mathbf{v}}{dt} + \mathbf{F}^T \otimes J(\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX,$$

leading to

$$\begin{aligned} \int_{\Omega_0} \text{tr}(\tilde{\boldsymbol{\Sigma}}^t) dX &\equiv \int_{\Omega_0} \boldsymbol{\Sigma} dX \\ &= -\langle \hat{V}_0 \rangle + \int_{\Omega_0} \mathbf{R} \cdot \left\{ \mathbf{F}^T \otimes \rho J \frac{d\mathbf{v}}{dt} + \mathbf{F}^T \otimes J(\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX. \end{aligned} \quad (5-4)$$

The averaged material virial therein satisfies the material version of the tensorial virial theorem (for asymptotic times), which is the equality

$$\langle \hat{V}_0 \rangle = \langle \hat{V}_{0\text{ext,tot}} \rangle + \langle \hat{V}_{0\text{int}} \rangle, \quad \langle \hat{V}_{0\text{ext,tot}} \rangle + \langle \hat{V}_{0\text{int}} \rangle + 2\langle \hat{\mathbf{E}}_k \rangle = \mathbf{0}. \quad (5-5)$$

This writing leads to the following expression of the average Eshelby stress

$$\begin{aligned} \bar{\boldsymbol{\Sigma}} &:= \frac{1}{|\Omega_0|} \int_{\Omega_0} \boldsymbol{\Sigma} dX \\ &= -\frac{1}{|\Omega_0|} \langle \hat{V}_0 \rangle + \frac{1}{|\Omega_0|} \int_{\Omega_0} \mathbf{R} \cdot \left\{ \mathbf{F}^T \otimes \rho J \frac{d\mathbf{v}}{dt} + \mathbf{F}^T \otimes J(\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX \\ &= \frac{1}{|\Omega_0|} \{ \langle \hat{V}_{0\text{int}} \rangle + 2\langle \mathbf{E}_k \rangle \} + \frac{1}{|\Omega_0|} \int_{\Omega_0} \mathbf{R} \cdot \left\{ \mathbf{F}^T \otimes \rho J \frac{d\mathbf{v}}{dt} + \mathbf{F}^T \otimes J(\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX, \end{aligned} \quad (5-6)$$

the right-hand side being evaluated using the discrete expression of the internal virial and kinetic energy (averaged over long times); the internal virial results from the additive decomposition of the total tensor virial into the internal and external virials,

$$\hat{V} = (\mathbf{r}_{ij} \otimes \mathbf{f}_{ij})_{j \neq i} + \mathbf{r}_i \otimes \mathbf{f}_{i,\text{ext}} \equiv \hat{V}_{\text{int}} + \hat{V}_{\text{ext}}, \quad (5-7)$$

which leads to

$$\hat{V}_{0\text{int}} \equiv (\mathbf{r}_{ij} \otimes \mathbf{F}^T \cdot \mathbf{f}_{ij})_{j \neq i},$$

adopting the following definition for the total discrete tensorial virial:

$$\hat{V}_0 = \sum_{i=1}^N \mathbf{R}_i \otimes \mathbf{F}^t \cdot \mathbf{f}_{0i}.$$

Expression (5-6) involves the pull-back to the material manifold of the referential internal (trading interactions between particles within the considered domain) forces $\mathbf{F}^t \cdot \mathbf{f}_{ij}$, accounting for both contact and volumetric forces.

Observe that the introduced fourth-order Eshelby tensor $\tilde{\tilde{\Sigma}}$ involved in previous derivations is an intermediate object originating from the mathematical developments initiated from the tensorial eulerian virial, which finally reduces to the classical (second order) Eshelby tensor by taking the trace of $\tilde{\tilde{\Sigma}}$.

The balance of momentum satisfied by the effective Eshelby stress

$$\tilde{\Sigma} := W\mathbf{I} - \mathbf{F}^T \cdot \tilde{\mathbf{T}}$$

, built from $\tilde{\mathbf{T}}$, is derived in [Appendix A](#), leading to equality (A-12), which is recalled for completeness:

$$\rho_R \mathbf{F}^T \cdot \frac{\partial \mathbf{v}}{\partial t} = \mathbf{f}_R + \Pi \mathbf{F}^T \cdot \mathbf{v} + \nabla_R \mathbf{F} : (\mathbf{J}_R \otimes \mathbf{v}) - \nabla_R \cdot \tilde{\Sigma} + (\partial_X \psi)_{\text{expl}}. \quad (5-8)$$

In (5-8), the quantity $\Pi \mathbf{F}^T \cdot \mathbf{v} + \mathbf{J}_R \cdot \nabla_R \mathbf{F} \cdot \mathbf{v} + \nabla_R \mathbf{F} : (\mathbf{J}_R \otimes \mathbf{v})$ reflecting mass production and mass flux would vanish for closed systems with constant mass, in addition to modified Eshelby stress $\tilde{\Sigma}$ coinciding with the classical Eshelby stress Σ .

6. Conclusion

We have derived formal expressions of the Cauchy and Eshelby stress tensors for continuum bodies with varying mass, a situation of interest for growing solid bodies or for gravitational masses subjected to accretion phenomena. The adopted methodology relies on an extension of the virial theorem to situations of non constant mass, traded by a mass flux through the system boundaries and a mass production term. These two additional contributions entail modifications of the balance of momentum, when considering either a spatial formulation involving Cauchy stress or a material formulation relying on Eshelby stress. The stress measures in both material and physical format have been expressed versus the tensorial virial, highlighting an additional contribution from the mass flux.

The present study shed some new light on the microscopic interpretation of Cauchy and Eshelby stress for systems with variable mass, bridging the gap between the microscopic (particle level) and the macroscopic continuum scales. Interpretation of those results from the microscopic or molecular point of view highlights

that stresses may identified as the average of the virial tensor with additional contributions arising from the mass flux of particles entering the system, their evaluation resulting from the solution of the (dynamical in general) equations of motion at the microscopic or atomic level. This strategy may prove a convenient way to evaluate Eshelby and Cauchy stresses from discrete quantities, such as in finite element calculations (numerical approximation of a continuum model) or in simulations involving a two scale approach, like mixed atomistic continuum formulations. This approach appears of great interest in nanoscale systems with varying number of atoms due, for instance, to epitaxial growth, based on the extensive use of molecular dynamical simulations to explore the behavior of systems of atoms and molecules.

Appendix A. Balance of momentum satisfied by the effective Eshelby stress

The material form of the mass balance equation writes [Epstein and Maugin 2000],

$$\frac{\partial \rho_R}{\partial t} = \Pi - \text{Div } \mathbf{J}_R \quad (\text{A-1})$$

with the Lagrangian source and mass fluxes, respectively quantities Π and \mathbf{J}_R , given versus their spatial counterparts as

$$\Pi = J\pi, \quad \mathbf{J} = J^{-1} \mathbf{F} \cdot \mathbf{J}_R \quad (\text{A-2})$$

with the Jacobian $J := \det(\mathbf{F})$. The Lagrangian balance of momentum expresses in terms of the nominal stress \mathbf{T} , the first Piola–Kirchhoff stress tensor, as

$$\rho_R \frac{\partial \mathbf{v}}{\partial t} = \mathbf{f} + \nabla_R \cdot \mathbf{T} - (\mathbf{J}_R \cdot \nabla_R) \mathbf{v} \quad (\text{A-3})$$

which rewrites accounting for the mass balance equation (A-1) as the dynamical equilibrium

$$\rho_R \frac{\partial \mathbf{v}}{\partial t} = \mathbf{f} + \Pi \mathbf{v} + \nabla_R \cdot (\mathbf{T} - \mathbf{J}_R \otimes \mathbf{v}). \quad (\text{A-4})$$

The balance of angular momentum expresses as the symmetry condition for the second-order tensor $\tilde{\mathbf{T}} := \mathbf{T} - \mathbf{J}_R \otimes \mathbf{v}$, called the effective first Piola–Kirchhoff stress.

The material version of the balance of momentum is obtained by a pull-back of the eulerian version, using the relations [Milstein 1982]

$$\text{Div}(J \mathbf{F}^{-T}) = \mathbf{0} \quad \Rightarrow \quad \nabla_R \cdot \mathbf{T} = J \nabla \cdot \boldsymbol{\sigma}, \quad (\text{A-5})$$

leading to

$$\begin{aligned} \rho_R \mathbf{F}^T \cdot \frac{\partial \mathbf{v}}{\partial t} &= \mathbf{F}^T \cdot \mathbf{f} + \Pi \mathbf{F}^T \cdot \mathbf{v} + \mathbf{F}^T \cdot \nabla_R \cdot \tilde{\mathbf{T}} \\ &= \mathbf{F}^T \cdot \mathbf{f} + \Pi \mathbf{F}^T \cdot \mathbf{v} + \mathbf{F}^T \cdot \nabla_R \cdot \mathbf{T} - \mathbf{F}^T \cdot \nabla_R \cdot (\mathbf{J}_R \otimes \mathbf{v}). \end{aligned} \quad (\text{A-6})$$

For a hyperelastic medium with strain energy density $W = W(\mathbf{F}; X)$, consideration of the following identity for the total spatial material derivative of W [Maugin 1993]

$$d_{X^A} W = \frac{\partial W}{\partial F_i^I} F_{I,A}^i + \left(\frac{\partial W}{\partial X^A} \right)_{\text{expl}} \equiv T_i^I F_{I,A}^i + \left(\frac{\partial W}{\partial X^A} \right)_{\text{expl}} \quad (\text{A-7})$$

leads to

$$\mathbf{F}^T \cdot \nabla_R \cdot \mathbf{T} = \nabla_R \cdot [\mathbf{F}^T \cdot \mathbf{T} - W \mathbf{I}] + (\partial_X W)_{\text{expl}}. \quad (\text{A-8})$$

Due further to the equality

$$\begin{aligned} \mathbf{F}^T \cdot \nabla_R \cdot (\mathbf{J}_R \otimes \mathbf{v}) &= \mathbf{F}^T \cdot \{ \mathbf{J}_R \cdot (\nabla_R \cdot \mathbf{v}) + \nabla_R \mathbf{J}_R \cdot \mathbf{v} \} \\ &= (\nabla_R \cdot \mathbf{v}) \mathbf{F}^T \cdot \mathbf{J}_R + \mathbf{F}^T \cdot \nabla_R \mathbf{J}_R \cdot \mathbf{v} \end{aligned} \quad (\text{A-9})$$

one easily obtains

$$\nabla_R \cdot [\mathbf{F}^T \cdot \tilde{\mathbf{T}} - W \mathbf{I}] = \nabla_R \cdot [\mathbf{F}^T \cdot \mathbf{T} - \mathbf{F}^T \cdot \mathbf{J}_R \otimes \mathbf{v} - W \mathbf{I}], \quad (\text{A-10})$$

with

$$\begin{aligned} (\mathbf{F}^T \cdot \tilde{\mathbf{T}})_{ij,j} &= (F_{ki} \tilde{T}_{kj})_{,j} = F_{ki,j} \tilde{T}_{kj} + F_{ki} \tilde{T}_{kj,j} \\ &= (F_{ki,j} T_{kj} + F_{ki} T_{kj,j}) - J_{Rk} F_{ki,j} v_j + F_{ki} (\nabla_R \cdot (\mathbf{J}_R \otimes \mathbf{v}))_{kj}, \end{aligned}$$

and hence the equality

$$-\nabla_R \cdot \tilde{\Sigma} = -\nabla_R \cdot \Sigma - \mathbf{J}_R \cdot \nabla_R \mathbf{F} \cdot \mathbf{v} - \nabla_R \cdot (\mathbf{F}^T \cdot (\mathbf{J}_R \otimes \mathbf{v}))$$

involving the Eshelby stress and modified Eshelby stress built from the hyperelastic potential W :

$$\Sigma := W \mathbf{I} - \mathbf{F}^T \cdot \mathbf{T}, \quad \tilde{\Sigma} := W \mathbf{I} - \mathbf{F}^T \cdot \tilde{\mathbf{T}}. \quad (\text{A-11})$$

More general similar derivations including chemical and thermal effects have been obtained in [Ganghoffer 2010b].

We further elaborate the dynamical equilibrium as

$$\begin{aligned} \rho_R \mathbf{F}^T \cdot \frac{\partial \mathbf{v}}{\partial t} &= \mathbf{F}^T \cdot \mathbf{f} + \Pi \mathbf{F}^T \cdot \mathbf{v} + \mathbf{F}^T \cdot \nabla_R \cdot \tilde{\mathbf{T}} \\ &\equiv \mathbf{F}^T \cdot \mathbf{f} + \Pi \mathbf{F}^T \cdot \mathbf{v} + \mathbf{F}^T \cdot \nabla_R \cdot \mathbf{T} - \mathbf{F}^T \cdot \nabla_R \cdot (\mathbf{J}_R \otimes \mathbf{v}), \\ \rho_R \mathbf{F}^T \cdot \frac{\partial \mathbf{v}}{\partial t} &= \mathbf{f}_R + \Pi \mathbf{F}^T \cdot \mathbf{v} - \nabla_R \cdot \Sigma + (\partial_X \psi)_{\text{expl}} - \mathbf{F}^T \cdot \nabla_R \cdot (\mathbf{J}_R \otimes \mathbf{v}), \end{aligned}$$

which is equivalent to

$$\begin{aligned} \rho_R \mathbf{F}^T \cdot \frac{\partial \mathbf{v}}{\partial t} \\ = \mathbf{f}_R + \Pi \mathbf{F}^T \cdot \mathbf{v} - \nabla_R \cdot \tilde{\Sigma} + (\partial_X \psi)_{\text{expl}} + \nabla_R \cdot \{ \mathbf{F}^T \cdot (\mathbf{J}_R \otimes \mathbf{v}) \} - \mathbf{F}^T \cdot \nabla_R \cdot (\mathbf{J}_R \otimes \mathbf{v}), \end{aligned}$$

or again to the equality

$$\rho_R \mathbf{F}^T \cdot \frac{\partial \mathbf{v}}{\partial t} = \mathbf{f}_R + \Pi \mathbf{F}^T \cdot \mathbf{v} - \nabla_R \cdot \tilde{\Sigma} + \nabla_R \mathbf{F} : (\mathbf{J}_R \otimes \mathbf{v}) + (\partial_X \psi)_{\text{expl}}, \quad (\text{A-12})$$

involving the referential body forces $\mathbf{f}_R := \mathbf{F}^T \cdot \mathbf{f}$. The modified effective Eshelby stress in (A-12) is the purely material stress incorporating the mass flux contribution.

Appendix B. Derivation of the average Eshelby stress from the virial theorem

The starting point is the relation (5-2), which is rewritten for the sake of clarity as

$$\langle \hat{V} \rangle \equiv \int_{\partial \Omega} \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} \, d\sigma_t + \int_{\Omega} \mathbf{r} \otimes \mathbf{f} \, dx. \quad (\text{B-1})$$

We then analyse the dyadic moment of physical forces—in the vocabulary of [Steinmann 2000]—therein:

$$\begin{aligned} \int_{\partial \Omega} \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{n} \, d\sigma_t &\equiv \int_{\partial \Omega} r_i \sigma_{jk} n_k \, d\sigma_t = \int_{\Omega} (r_i \sigma_{jk})'_{,k} \, dx = \int_{\Omega} (r_i'_{,k} \sigma_{jk} + r_i \sigma_{jk,k}) \, dx \\ &\equiv \int_{\Omega} (\text{grad } \mathbf{r} \cdot \boldsymbol{\sigma}^T + \mathbf{r} \otimes \text{div } \boldsymbol{\sigma}) \, dx \\ &= \int_{\Omega} \mathbf{I} \cdot \boldsymbol{\sigma}^T \, dx + \int_{\Omega} \mathbf{r} \otimes \text{div } \boldsymbol{\sigma} \, dx. \end{aligned} \quad (\text{B-2})$$

Hence, assembling both contributions in $\langle \hat{V} \rangle$ gives

$$\langle \hat{V} \rangle \equiv \int_{\Omega} \mathbf{I} \cdot \mathbf{J} \boldsymbol{\sigma}^T \, dX + \int_{\Omega_0} \mathbf{R} \cdot \{ \mathbf{F}^T \otimes \mathbf{J} \text{div } \boldsymbol{\sigma} + \mathbf{F}^T \otimes \mathbf{f}_0 \} \, dX \quad (\text{B-3})$$

recalling that $\mathbf{f}_0 := \mathbf{J} \mathbf{f}$.

A material form of static equilibrium shall next be expressed, obtained by transforming the integrand in (B-3) in a Lagrangian format. As a first step, the identity

$$\mathbf{F}^T \otimes \text{Div } \mathbf{T} = \text{Div}(\mathbf{F}^T \otimes \mathbf{T}) - \text{Grad}(W_0 \mathbf{I}) \quad (\text{B-4})$$

is easily obtained, with

$$\text{Grad}(W_0 \mathbf{I}) = \text{Grad } \mathbf{F}^T \cdot \mathbf{T} \equiv (\mathbf{F}^t)_{Ai,B} T_{jB},$$

the contraction being done on the material subscript B ; observe that this relation is the tensorial generalization of the identity

$$\text{Div}(W_0 \mathbf{I}) = \text{Div } \mathbf{F}^T \cdot \mathbf{T}.$$

Let us further express the gradient $\text{Grad}(W \mathbf{I})$ above as the material divergence of

a fourth-order tensor: due to the equality

$$\mathbf{I}_4 : \mathbf{A} = \text{Tr}(\mathbf{A})\mathbf{I}$$

there follows the identity [Ganghoffer 2010b]

$$\text{Div}(W_0\mathbf{I}^4) = \text{Grad}(W_0\mathbf{I}). \quad (\text{B-5})$$

Let Div denote the material divergence, not to be confused with the spatial divergence operator, ∇ . From the classical Piola identity [Maugin 1993]

$$\text{div}(\mathbf{J}\mathbf{F}^{-T}) = \mathbf{0}$$

there follows further the relation)

$$\mathbf{J}\nabla \cdot \tilde{\boldsymbol{\sigma}}^T = \text{Div} \tilde{\mathbf{T}}^T$$

, with

$$\tilde{\mathbf{T}} = \mathbf{J}\tilde{\boldsymbol{\sigma}} \cdot \mathbf{F}^{-T} \equiv \mathbf{T} - \mathbf{J}(\mathbf{J} \otimes \mathbf{v}) \cdot \mathbf{F}^{-T} \quad (\text{B-6})$$

the effective first Piola–Kirchhoff stress tensor. Combining the last identities with the Eulerian balance of linear momentum (3-5) yields

$$\rho\mathbf{J}\frac{d\mathbf{v}}{dt} = (\mathbf{J}\mathbf{f} + \mathbf{v}\mathbf{J}\text{div} \mathbf{J}) + \mathbf{J}\nabla \cdot \tilde{\boldsymbol{\sigma}}^T,$$

which is to say

$$\rho\mathbf{J}\frac{d\mathbf{v}}{dt} = \tilde{\mathbf{f}}_0 + \text{Div} \tilde{\mathbf{T}}^T, \quad (\text{B-7})$$

with $\tilde{\mathbf{f}}_0 := (\mathbf{f}_0 + \mathbf{v}\mathbf{J}\text{div} \mathbf{J})$ the effective body forces, and recalling the expression $\tilde{\boldsymbol{\sigma}} := \boldsymbol{\sigma} - \mathbf{v} \otimes \mathbf{J}$ of the effective Cauchy stress.

The balance of linear momentum, (B-7), is further elaborated as

$$\mathbf{F}^T \otimes \rho\mathbf{J}\frac{d\mathbf{v}}{dt} = \mathbf{F}^T \otimes \tilde{\mathbf{f}}_0 + \mathbf{F}^T \otimes \text{Div} \tilde{\mathbf{T}}^T.$$

Due further to the relation satisfied by the (classical) first Piola–Kirchhoff stress tensor,

$$\mathbf{F}^T \otimes \text{Div} \mathbf{T} = \text{Div}(\mathbf{F}^T \otimes \mathbf{T}) - \text{Grad}(W_0\mathbf{I}) \equiv \text{Div}(\mathbf{F}^T \otimes \mathbf{T} - W_0\mathbf{I}^4),$$

there follows the dynamical tensorial equilibrium equation

$$\mathbf{F}^T \otimes \rho\mathbf{J}\frac{d\mathbf{v}}{dt} = \mathbf{F}^T \otimes \tilde{\mathbf{f}}_0 - \text{Div} \tilde{\tilde{\boldsymbol{\Sigma}}} - \mathbf{F}^T \otimes \text{Div}\{ \mathbf{J}(\mathbf{J} \otimes \mathbf{v}) \cdot \mathbf{F}^{-T} \} \quad (\text{B-8})$$

involving the fourth-order material Eshelby tensor (denoted by a double tilde)

$$\tilde{\tilde{\boldsymbol{\Sigma}}} := W_0\mathbf{I}^4 - \mathbf{F}^T \otimes \mathbf{T}.$$

Adopting

$$\text{tr}(A \otimes B) := A \cdot B, \quad \forall A, B$$

as the definition of the trace of a fourth-order tensor built as the dyadic product of two second-order tensors, the trace of the fourth-order Eshelby tensor yields the second-order Eshelby tensor

$$\Sigma := W_0 I - F^T \cdot T.$$

It is easy to show that Σ satisfies the following dynamical balance of linear momentum incorporating the mass flux:

$$\rho J F^T \cdot \frac{dv}{dt} = F^T \cdot \tilde{f}_0 - \text{Div } \Sigma - F^T \cdot \text{Div}\{J(J \otimes v) \cdot F^{-T}\}. \quad (\text{B-9})$$

The previous implications also show the identities

$$F^t \otimes J \text{div } \sigma + F^t \otimes f_0 \equiv F^t \text{Div } T + F^t \otimes f_0 = -\text{Div } \tilde{\Sigma} + F^t \otimes f_0. \quad (\text{B-10})$$

Inserting this back into the tensorial eulerian virial further delivers

$$\begin{aligned} \langle \hat{V} \rangle &\equiv \int_{\Omega_0} I \cdot J \sigma^T dX + \int_{\Omega_0} R \cdot \{F^T \otimes J \text{div } \sigma + F^T \otimes f_0\} dX \\ &\equiv \int_{\Omega_0} I \cdot J \sigma^T dX + \int_{\Omega_0} R \cdot \{-\text{Div } \tilde{\Sigma} + F^T \otimes f_0\} dX. \end{aligned}$$

Taking into account the eulerian form of the dynamical equilibrium, expressed as

$$\nabla \cdot \sigma = \rho \frac{dv}{dt} - f + (J \cdot \nabla) v,$$

one obtains

$$\begin{aligned} \langle \hat{V} \rangle &\equiv \int_{\Omega_0} I \cdot J \sigma^T dX + \int_{\Omega_0} R \cdot \left\{ F^T \otimes J \left[\rho \frac{dv}{dt} - f + (J \cdot \nabla) v \right] + F^T \otimes f_0 \right\} dX \\ &\equiv \int_{\Omega_0} I \cdot J \sigma^T dX \\ &\quad + \int_{\Omega_0} R \cdot \left\{ -\text{Div } \tilde{\Sigma} - F^T \otimes \text{Div}\{J(J \otimes v) \cdot F^{-T}\} + (J \cdot \nabla) v + F^T \otimes f_0 \right\} dX. \end{aligned}$$

Further, the elaboration of Eshelby stress in terms of Cauchy stress is expressed by

$$\Sigma = W_0 I - J F^T \cdot \sigma \cdot F^{-T},$$

or equivalently

$$\sigma = -j F^{-T} \cdot \Sigma \cdot F^T + W_t I,$$

observing that the product jW_0 represents the density of strain energy in the current configuration:

$$W_t := jW_0.$$

This leads to a rewriting of the averaged Cauchy stress in terms of the Eshelby stress:

$$\int_{\Omega} (\boldsymbol{\sigma}^T \cdot \mathbf{I}) dx = \int_{\Omega_0} J \boldsymbol{\sigma}^T \cdot \mathbf{I} dX = \int_{\Omega_0} (-\mathbf{F}^{-T} \cdot \boldsymbol{\Sigma} \cdot \mathbf{F}^T + W_0 \mathbf{I}) dX.$$

Hence, the previous form of the tensorial eulerian virial becomes, after lengthy developments,

$$\begin{aligned} \langle \hat{V} \rangle &\equiv \int_{\Omega_0} (-\mathbf{F}^{-t} \cdot \boldsymbol{\Sigma} \cdot \mathbf{F}^t + W_0 \mathbf{I}) dX + \int_{\Omega_0} \mathbf{R} \cdot \{-\text{Div} \tilde{\boldsymbol{\Sigma}} + \mathbf{F}^t \otimes \mathbf{f}_0\} dX \\ &\equiv \int_{\Omega_0} (-\mathbf{F}^{-t} \cdot \boldsymbol{\Sigma} \cdot \mathbf{F}^t + W_0 \mathbf{I}) dX, \\ \langle \hat{V} \rangle &\equiv \int_{\Omega_0} \mathbf{I} \cdot J \boldsymbol{\sigma}^T dX + \int_{\Omega_0} \mathbf{R} \cdot \left\{ \mathbf{F}^T \otimes J \left\{ \rho \frac{d\mathbf{v}}{dt} - \mathbf{f} + (\mathbf{J} \cdot \nabla) \mathbf{v} \right\} + \mathbf{F}^T \otimes \mathbf{f}_0 \right\} dX \\ &\equiv \int_{\Omega_0} (-\mathbf{F}^{-T} \cdot \boldsymbol{\Sigma} \cdot \mathbf{F}^T + W_0 \mathbf{I}) dX \\ &\quad + \int_{\Omega_0} \mathbf{R} \cdot \left\{ -\text{Div} \tilde{\boldsymbol{\Sigma}} + \mathbf{F}^T \otimes \mathbf{f}_0 + \mathbf{F}^T \otimes J \rho \frac{d\mathbf{v}}{dt} \right. \\ &\quad \left. - \mathbf{F}^T \otimes \text{Div} \{ J(\mathbf{J} \otimes \mathbf{v}) \cdot \mathbf{F}^{-T} \} + (\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX \\ &= \int_{\Omega_0} (-\text{tr}(\tilde{\boldsymbol{\Sigma}}^t) + W_0 \mathbf{I}) dX \\ &\quad + \int_{\Omega_0} \mathbf{R} \cdot \left\{ -\text{Div} \tilde{\boldsymbol{\Sigma}} + \mathbf{F}^T \otimes \mathbf{f}_0 \right. \\ &\quad \left. - \mathbf{F}^T \otimes \text{Div} \{ J(\mathbf{J} \otimes \mathbf{v}) \cdot \mathbf{F}^{-T} \} + \mathbf{F}^T \otimes J(\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX \\ &\equiv \int_{\Omega_0} (-\text{tr}(\tilde{\boldsymbol{\Sigma}}^t) + W_0 \mathbf{I}) dX + \int_{\Omega_0} \mathbf{R} \cdot \left\{ \mathbf{F}^T \otimes \rho J \frac{d\mathbf{v}}{dt} + \mathbf{F}^T \otimes J(\mathbf{J} \cdot \nabla) \mathbf{v} \right\} dX. \end{aligned}$$

Here we have taken into account the static equilibrium and the identity

$$\begin{aligned} \int_{\Omega_0} (-\mathbf{F}^{-t} \cdot \boldsymbol{\Sigma} \cdot \mathbf{F}^t + W_0 \mathbf{I}) dX &\equiv \int_{\Omega_0} (-\boldsymbol{\Sigma}^t + W_0 \mathbf{I}) dX \\ &= \int_{\Omega_0} (-\text{tr}(\tilde{\boldsymbol{\Sigma}}^t) + W_0 \mathbf{I}) dX, \end{aligned} \quad (\text{B-11})$$

itself resulting from the equality

$$(\mathbf{A} \otimes \mathbf{B})^T = \mathbf{B} \otimes \mathbf{A}, \quad \forall \mathbf{A}, \mathbf{B},$$

the coaxiality of \mathbf{T} with \mathbf{F}^t [Ciarlet 1993], and the following definition of the trace of a fourth-order tensor built as the dyadic product of two second-order tensors:

$$\text{tr}(\mathbf{A} \otimes \mathbf{B}) := \mathbf{A} \cdot \mathbf{B}, \quad \forall \mathbf{A}, \mathbf{B}.$$

According to this definition, the trace of the fourth-order Eshelby tensor in delivers the second-order Eshelby tensor.

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